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NEWS 4 OCT 07 Multiple databases enhanced for more flexible patent
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NEWS 5 OCT 22 Current-awareness alert (SDI) setup and editing
enhanced
NEWS 6 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
Applications
NEWS 7 OCT 24 CHEMLIST enhanced with intermediate list of
pre-registered REACH substances
NEWS 8 NOV 21 CAS patent coverage to include exemplified prophetic
substances identified in English-, French-, German-,
and Japanese-language basic patents from 2004-present
NEWS 9 NOV 26 MARPAT enhanced with FSORT command
NEWS 10 NOV 26 MEDLINE year-end processing temporarily halts
availability of new fully-indexed citations
NEWS 11 NOV 26 CHEMSAFE now available on STN Easy
NEWS 12 NOV 26 Two new SET commands increase convenience of STN
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NEWS 13 DEC 01 ChemPort single article sales feature unavailable
NEWS 14 DEC 12 GBFULL now offers single source for full-text
coverage of complete UK patent families
NEWS 15 DEC 17 Fifty-one pharmaceutical ingredients added to PS

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 14:11:05 ON 18 DEC 2008

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COST IN U.S. DOLLARS
FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 14:12:01 ON 18 DEC 2008
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DICTIONARY FILE UPDATES: 17 DEC 2008 HIGHEST RN 1086212-50-1

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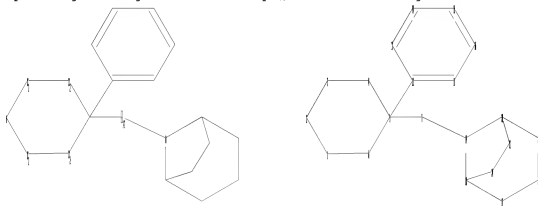
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=>
Uploading C:\Program Files\Stnexp\Queries\10-538144genC.str



chain nodes :
7
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16 17 18 19 20 21 22 23 24
chain bonds :
5-7 5-12 7-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22
18-19 18-24 19-20 20-21 20-23 21-22 23-24
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-19 17-18 17-22 18-19 18-24 19-20 20-21 20-23
21-22 23-24
exact bonds :

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normalized bonds :
11-12 11-16 12-13 13-14 14-15 15-16

G1:Cb,Cy,Hy,Ak

Match level :

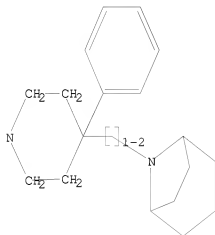
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14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 14:13:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1834 TO ITERATE

100.0% PROCESSED 1834 ITERATIONS

1261 ANSWERS

SEARCH TIME: 00.00.01

L2 1261 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

182.96

183.38

FILE 'CAPLUS' ENTERED AT 14:18:38 ON 18 DEC 2008

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FILE COVERS 1907 - 18 Dec 2008 VOL 149 ISS 25
FILE LAST UPDATED: 17 Dec 2008 (20081217/ED)

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=> s l2
L3

2 L2

=> d l2 1-2 abs ibib hitstr
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d l3 1-2 abs ibib hitstr

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

AB We describe robust chemical approaches toward putative CCR5 scaffolds designed in our labs. Evaluation of analogs in the 125I-[MIP-1 β] binding and Ba-L-HOS antiviral assays resulted in the discovery of 64 and 68 in the 4,4-disubstituted piperidine class H, both potent CCR5 ligands (pIC50 = 8.30 and 9.00, resp.) and HIV-1 inhibitors (pIC50 = 7.80 and 7.84, resp., in Ba-L-HOS assay). In addition, 64 and 68 were bioavailable in rodents, establishing them as lead mols. for further optimization toward CCR5 clin. candidates.

ACCESSION NUMBER: 2008:1154437 CAPLUS <<LOGINID::20081218>>

DOCUMENT NUMBER: 149:486141

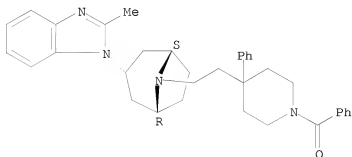
TITLE: Discovery of Bioavailable 4,4-Disubstituted Piperidines as Potent Ligands of the Chemokine Receptor 5 and Inhibitors of the Human Immunodeficiency Virus-1

AUTHOR(S): Kazmierski, Wieslaw M.; Aquino, Christopher; Chauder, Brian A.; Deanda, Felix; Ferris, Robert; Jones-Hertzog, Deborah K.; Kenakin, Terrence; Koble, Cecilia S.; Watson, Christian; Wheelan, Pat; Yang, Hanbiao; Youngman, Michael

CORPORATE SOURCE: Infectious Diseases Center for Excellence in Drug Discovery, Molecular Discovery Research, Computational and Structural Chemistry, Drug Discovery, IT ID DMPK, Metabolic Pathways Center for Excellence in Drug Discovery, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA

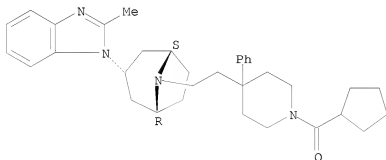
SOURCE: Journal of Medicinal Chemistry (2008), 51(20),
6538-6546
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 716344-87-5P 716344-88-6P 717101-60-5P
717101-63-8P 1071993-49-1P 1071993-56-0P
1072196-30-5P 1072196-31-6P 1072196-32-7P
1072196-33-8P 1072196-34-9P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
PREP (Preparation); USES (Uses)
(preparation of bioavailable piperidines as CCR5 ligands and HIV-1
inhibitors)
RN 716344-87-5 CAPLUS
CN Methanone, [4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-
azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]phenyl- (CA INDEX
NAME)

Relative stereochemistry.



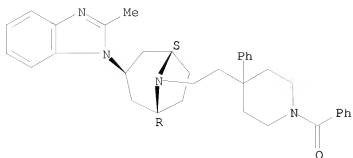
RN 716344-88-6 CAPLUS
CN Methanone, cyclopentyl[4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-
azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]- (CA INDEX NAME)

Relative stereochemistry.



RN 717101-60-5 CAPLUS
CN Methanone, [4-[2-[(3-exo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-
azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-1-piperidinyl]phenyl- (CA INDEX
NAME)

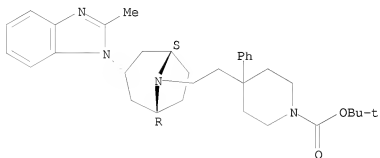
Relative stereochemistry.



RN 717101-63-8 CAPLUS

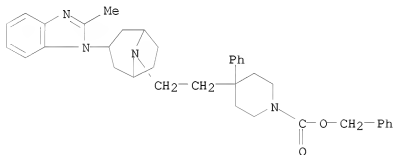
CN 1-Piperidinecarboxylic acid, 4-[2-[(3-endo)-3-(2-methyl-1H-benzimidazol-1-yl)-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

Relative stereochemistry.



RN 1071993-49-1 CAPLUS

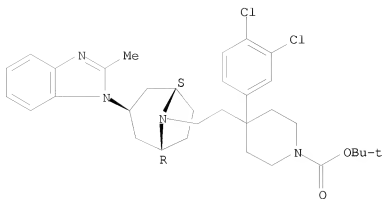
CN INDEX NAME NOT YET ASSIGNED



RN 1071993-56-0 CAPLUS

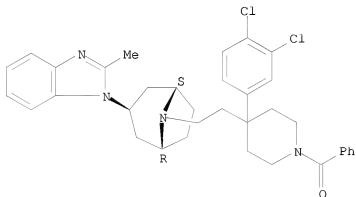
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



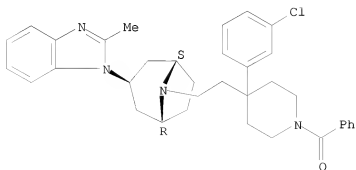
RN 1072196-30-5 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



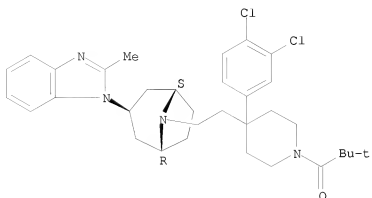
RN 1072196-31-6 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



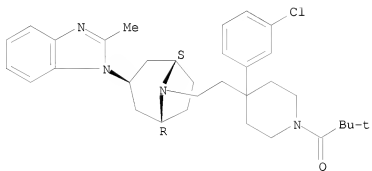
RN 1072196-32-7 CAPLUS
 CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



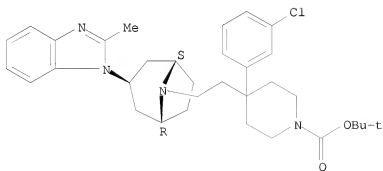
RN 1072196-33-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



RN 1072196-34-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.



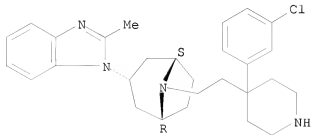
IT 716358-41-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bioavailable piperidines as CCR5 ligands and HIV-1 inhibitors)

RN 716358-41-7 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[2-[4-(3-chlorophenyl)-4-piperidinyl]ethyl]-3-(2-methyl-1H-benzimidazol-1-yl)-, hydrochloride (1:2), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



● 2 HCl

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl, heteroarylcyκλοalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocabonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cyanoimino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl, amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethiyl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic ring with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention

comps. have pIC50 values of ≥ 5 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarboxitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxyborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II.

ACCESSION NUMBER: 2004:534173 CAPLUS <<LOGINID:20081218>>
DOCUMENT NUMBER: 141:89016
TITLE: Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection
INVENTOR(S): Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil; Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vandervall, Dana
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; et al.; et al.
SOURCE: PCT Int. Appl., 859 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054974	A2	20040701	WO 2003-US39644	20031212
WO 2004054974	A3	20040902		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2509711	A1	20040701	CA 2003-2509711	20031212
AU 2003300902	A1	20040709	AU 2003-300902	20031212
EP 1569646	A2	20050907	EP 2003-813419	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017230	A	20051025	BR 2003-17230	20031212
CN 1744899	A	20060308	CN 2003-80109628	20031212
JP 2006511554	T	20060406	JP 2004-560838	20031212
NO 2005002739	A	20050819	NO 2005-2739	20050607
US 20060229336	A1	20061012	US 2005-538144	20050609
MX 2005PA06354	A	20050826	MX 2005-PA6354	20050613
IN 2005KN01328	A	20060630	IN 2005-KN1328	20050711

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			WO 2003-US39644	W 20031212

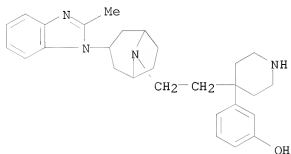
OTHER SOURCE(S): MARPAT 141:89016
 IT 1055923-67-5 1055923-68-6 1055923-71-1
 1055923-72-2 1055923-73-3

RL: PRPH (Prophetic)

(Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection)

RN 1055923-67-5 CAPLUS

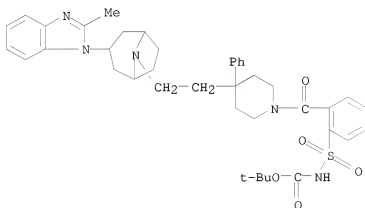
CN INDEX NAME NOT YET ASSIGNED



● HBr

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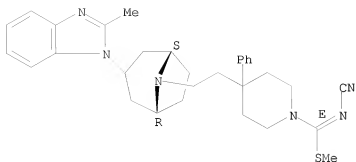
CN INDEX NAME NOT YET ASSIGNED



RN 1055923-71-1 CAPLUS

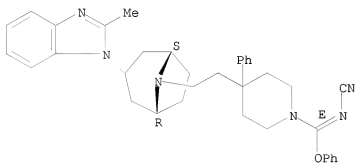
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
 Double bond geometry as shown.

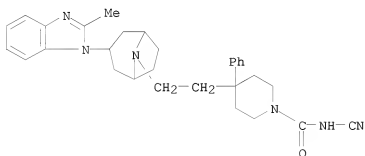


RN 1055923-72-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.
Double bond geometry as shown.



RN 1055923-73-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



IT 716344-72-8P 716344-76-2P 716344-78-4P
716344-80-8P 716344-82-0P 716344-84-2P
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716349-53-0P 716349-70-1P 716350-01-5P
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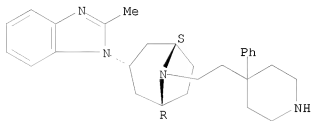
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RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of benzimidazolylazabicyclooctylethylpiperidine Ccr5 antagonists in treatment of bacterial and viral infections and other diseases)

RN 716344-72-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-(2-methyl-1H-benzimidazol-1-yl)-8-[2-(4-phenyl-4-piperidiny)ethyl]-, hydrochloride (1:2), (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



● 2 HCl